

On extremal trees with respect to the F -index

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Abstract

In a study on the structure–dependency of the total π -electron energy from 1972, Trinajstić and one of the present authors have shown that it depends on the sums $\sum_{v \in V} d(v)^2$ and $\sum_{v \in V} d(v)^3$, where $d(v)$ is the degree of a vertex v of the underlying molecular graph G . The first sum was later named *first Zagreb index* and over the years became one of the most investigated graph–based molecular structure descriptors. On the other hand, the second sum, except in very few works on the general first Zagreb index and the zeroth–order general Randić index, has been almost completely neglected. Recently, this second sum was named *forgotten index*, or shortly the F -index, and shown to have an exceptional applicative potential. In this paper we examine the trees extremal with respect to the F -index.

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1 Introduction

The first and the second Zagreb indices, introduced in 1972 [16], are among the oldest graph-based molecular structure descriptors, so-called topological indices [1, 8, 11]. For a graph G with a vertex set $V(G)$ and an edge set $E(G)$, these are defined as

$$M_1(G) = \sum_{v \in V(G)} d(v)^2 \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v),$$

where the degree of a vertex $v \in V(G)$, denoted by $d(v)$, is the number of the first neighbors of v .

Over the years these indices have been thoroughly examined and used to study molecular complexity, chirality, ZE-isomerism and hetero-systems. More about their physico-chemical applications and mathematical properties can be found in [10, 11, 24] and [6, 13, 14, 21, 30], respectively, as well as in the references cited therein. The sum of squares of vertex degrees was also independently studied in quite a few mathematical papers [2–5, 7, 25].

In an early work on the structure-dependency of the total π -electron energy [16], beside the first Zagreb index, it was indicated that another term on which this energy depends is of the form

$$F(G) = \sum_{v \in V(G)} d(v)^3.$$

For unexplainable reasons, the above sum, except (implicitly) in a few works about the general first Zagreb index [19, 20] and the zeroth-order general Randić index [17], has been completely neglected. Very recently, Furtula and one of the present authors succeeded to demonstrate that $F(G)$ has a very promising applicative potential [9]. They proposed that $F(G)$ be named the *forgotten topological index*, or shortly the *F-index*.

Before the publication of the paper [9], the F -index was not examined as such. On the other hand, in some earlier studies on degree-based graph invariants, it appears as a special case.

The *general first Zagreb index* of a graph G is defined as

$$M_1^\alpha(G) = \sum_{v \in V(G)} d(v)^\alpha = \sum_{uv \in E(G)} [d(u)^{\alpha-1} + d(v)^{\alpha-1}], \quad \text{for } \alpha \in \mathbb{R}, \alpha \neq 0, \alpha \neq 1,$$

and its first occurrence in the literature seems to be the work [19] by Li and Zhao from 2004. Observe that $M_1^3(G) = F(G)$. In [19] the trees with the first three smallest and largest general first Zagreb index were characterized. In [19, 20], among other things, it was shown that for $\alpha > 1$, the star S_n is the tree on n vertices with maximal M_1^α whereas the path P_n is the tree on n vertices with minimal M_1^α -value. Needless to say that these results directly apply to the F -index ($\alpha = 3$). More results and information about the general first Zagreb index can be found in [12, 17, 19, 20, 22, 28, 29].

The *Randić (or connectivity)* index was introduced by Randić in 1975 [27] and is defined as

$$R = R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}.$$

Later in 1977, Kier and Hall [18] have introduced the so-called *zeroth-order Randić index*

$${}^0R = {}^0R(G) = \sum_{v \in V(G)} d(v)^{-\frac{1}{2}},$$

which was generalized in 2005 by Li and Zheng [20]. It was named the *zeroth-order general Randić index* and was defined as

$${}^0R_\alpha = {}^0R_\alpha(G) = \sum_{v \in V(G)} d(v)^\alpha$$

for any real number α . Evidently, ${}^0R_3(G) = F(G)$.

In [17] graphs of maximal degree at most 4 (molecular graphs), with given number of vertices and edges, and with extremal (maximum or minimum) zeroth-order general Randić index were characterized. This, again, in the special case $\alpha = 3$ renders results for the F -index.

Here, we extend the work on trees with extremal values of F -index, by considering trees with bounded maximal degree. Since the paths are the trees with minimal F -index also in this case, we consider here the characterization of trees with bounded maximal degree that have maximal F -value.

In the sequel we introduce notation that will be used in the rest of the paper. For $u, v, x, y \in V(G)$ such that $uv \in E(G)$, $xy \notin E(G)$, we denote by $G - uv$ the graph that is obtained by deleting the edge uv from G and by $G + xy$ the graph that is obtained by adding the edge xy to G . By $\Delta = \Delta(G)$ we denote the maximal

degree of G . A sequence $D = [d_1, d_2, \dots, d_n]$ is *graphical* if there is a graph whose vertex degrees are d_i , $i = 1, \dots, n$. If in addition $d_1 \geq d_2 \geq \dots \geq d_n$, then D is a *degree sequence*. Furthermore, the notation $D(G) = [x_1^{n_1}, x_2^{n_2}, \dots, x_t^{n_t}]$ means that the degree sequence is comprised of n_i vertices of degree x_i , where $i = 1, 2, \dots, t$.

A tree is said to be *rooted* if one of its vertices has been designated as the *root*. In a rooted tree, the *parent* of a vertex is the vertex adjacent to it on the path to the root; every vertex except the root has a unique parent. A vertex is a parent of a subtree, if this subtree is attached to the vertex. A *child* of a vertex v is a vertex of which v is the parent.

2 Results

First, we characterize trees with maximal degree at most Δ that have maximal F -index.

2.1 Trees with bounded maximal degree

Theorem 2.1. *Let T be a tree with maximal F -index among the trees with n vertices and maximal degree at most Δ . Then the following holds:*

- (i) *If $(n - 2) \bmod (\Delta - 1) = 0$, then T contains $\frac{n-2}{\Delta-1}$ vertices of degree Δ and $\frac{n(\Delta-2)+2}{\Delta-1}$ vertices of degree 1.*
- (ii) *Otherwise, T contains $\frac{n-1-x}{\Delta-1}$ vertices of degree Δ , $\frac{(n-1)(\Delta-2)+x}{\Delta-1}$ vertices of degree 1 and one vertex of degree x , where x is uniquely determined by $2 \leq x \leq \Delta - 1$ and $(n - 1 - x) \bmod (\Delta - 1) = 0$.*

Proof. We may assume that T is a rooted tree, whose root is a vertex with degree Δ . First, we show that T is comprised of vertices of degrees Δ and 1, and in some cases of one additional vertex u , with $2 \leq d(u) \leq \Delta - 1$. Assume that this is not true and that T has more than one such vertex. Denote by V_d the set of all vertices of T whose degrees are different from Δ and 1. We assume that for the degrees of the vertices of V_d the order $d(u) \geq \dots \geq d(v)$ holds. Let w be a child vertex of v .

Delete the edge vw and add the edge uw to T , obtaining a tree T' . After this transformation, the degree of u increases by one, while the degree of v decreases by one, and the degree set V_d changed into V'_d . It holds that

$$F(T') - F(T) = (d(u) + 1)^3 - d(u)^3 + (d(w) - 1)^3 - d(w)^3 > 0.$$

It holds that $|V'_d| \leq |V_d|$, with strict inequality if $d(u) = \Delta - 1$ or $d(v) = 2$. If $|V'_d| \geq 2$ we choose from V'_d a vertex with maximal and a vertex with minimal degree, and we repeat the above operation, obtaining a tree with larger F -index. We proceed on iteratively with the same type of transformation until the transformed V_d has cardinality 1 or 0, and thus obtain a contradiction to the assumption that T has more than one vertex with degree different from 1 and Δ . It follows that T has a degree sequence $[\Delta^{n_\Delta}, 1^{n_1}]$ or $[\Delta^{n_\Delta}, x^1, 1^{n_1}]$, $2 \leq x \leq \Delta - 1$.

Observe that any transformation on T will result in a tree with $|V_d| > 1$ or will disconnect T . Thus, we conclude that T must have one of the two above presented degree sequences.

Next, with respect to the cardinality of $|V_d|$, we determine the parameters n_Δ , n_1 , and x .

Case 1. $|V_d| = 0$. In this case the degree sequence of T is $[\Delta^{n_\Delta}, 1^{n_1}]$ where the equations

$$\sum_{i=1}^{\Delta} n_i = n_\Delta + n_1 = n \quad \text{and} \quad \sum_{i=1}^{\Delta} i n_i = \Delta n_\Delta + n_1 = 2(n - 1)$$

hold. The above equations have the integer solution

$$n_\Delta = \frac{n - 2}{\Delta - 1}, \quad n_1 = \frac{n(\Delta - 2) + 2}{\Delta - 1},$$

for $(n - 2) \bmod (\Delta - 1) = 0$.

Case 2. $|V_d| = 1$. Here the degree sequence of T is $[\Delta^{n_\Delta}, x^1, 1^{n_1}]$, with

$$\sum_{i=1}^{\Delta} n_i = n_\Delta + n_1 + 1 = n \quad \text{and} \quad \sum_{i=1}^{\Delta} i n_i = \Delta n_\Delta + n_1 + x = 2(n - 1).$$

The above equations give the integer solution

$$n_\Delta = \frac{n - 1 - x}{\Delta - 1}, \quad n_1 = \frac{(n - 1)(\Delta - 2) + x}{\Delta - 1},$$

for $(n - 1 - x) \bmod (\Delta - 1) = 0$. □

As straightforward consequence of Theorem 2.1, we obtain the maximal value of the F -index for trees with maximal degree Δ .

Corollary 2.1. *Let T be a tree with maximal F -index among the trees with n vertices and maximal degree at most Δ . Then,*

(i) *if $(n - 2) \bmod (\Delta - 1) = 0$,*

$$F(T) = \Delta(\Delta + 1)(n - 2) + 2(n - 1);$$

(ii) *otherwise,*

$$F(T) = (\Delta^2 + \Delta + 2)(n - 1) - (\Delta^2 + \Delta + 1)x + x^3,$$

where x is uniquely determined by $2 \leq x \leq \Delta - 1$ and $n - 1 - x \bmod (\Delta - 1) = 0$.

Proof. If $(n - 2) \bmod (\Delta - 1) = 0$, by Theorem 2.1, T has degree sequence $[\Delta^{n_\Delta}, 1^{n_1}]$, where $n_\Delta = (n - 2)/(\Delta - 1)$ and $n_1 = (n(\Delta - 2) + 2)/(\Delta - 1)$. Thus,

$$F(T) = \Delta^3 \frac{n - 2}{\Delta - 1} + \frac{n(\Delta - 2) + 2}{\Delta - 1} = \Delta(\Delta + 1)(n - 2) + 2(n - 1).$$

Otherwise, T has degree sequence $[\Delta^{n_\Delta}, x^1, 1^{n_1}]$, where $n_\Delta = (n - 1 - x)/(\Delta - 1)$, $n_1 = ((n - 1)(\Delta - 2) + x)/(\Delta - 1)$. Then,

$$\begin{aligned} F(T) &= \Delta^3 \frac{n - (x + 1)}{\Delta - 1} + \frac{(n - 1)(\Delta - 2) + x}{\Delta - 1} + x^3 \\ &= \frac{(\Delta^3 + \Delta - 2)n + (1 - \Delta^3)x - (\Delta^3 + \Delta - 2)}{\Delta - 1} + x^3 \\ &= (\Delta^2 + \Delta + 2)(n - 1) - (\Delta^2 + \Delta + 1)x + x^3. \end{aligned}$$

□

2.2 Molecular trees

For the special case of molecular trees, i.e., $\Delta \leq 4$, we obtain the following result. Recall that such trees provide the graph representation of the so-called saturated hydrocarbons or alkanes [1, 15] and are of major importance in theoretical chemistry.

Theorem 2.2. *Let T be a molecular tree with maximal F -index among the trees with n vertices. Then the following holds:*

- If $(n-2) \bmod 3 = 0$, then T contains $\frac{n-2}{3}$ vertices of degree 4 and $\frac{2n+2}{3}$ vertices of degree 1. Its F -index is

$$F(T) = 22n - 42.$$

- Otherwise, T contains $\frac{n-1-x}{3}$ vertices of degree 4, $\frac{2(n-1)+x}{3}$ vertices of degree 1 and one vertex of degree x , where x is uniquely determined by $2 \leq x \leq 3$ and $(n-1-x) \bmod 3 = 0$. Its F -index is

$$F(T) = 22(n-1) - 21x + x^3.$$

Proof. For $n = 2, 3, 4, 5$ the star S_n maximizes the F -index [19]. For $n = 6$ and $\Delta \leq 4$, the possible degree sequences of T are $(4, 2, 1, 1, 1, 1)$, $(3, 3, 1, 1, 1, 1)$, $(3, 2, 2, 1, 1, 1)$ and $(2, 2, 2, 2, 1, 1)$. The first of these degree sequences corresponds to the largest F -index, $F(T)$.

Thus, the corresponding degree sequences of T for $n = 2, 3, 4, 5, 6$ satisfy the theorem.

In the rest of the proof we assume that $n \geq 7$. First, we show that T has maximal degree $\Delta = 4$. A tree with maximal degree Δ we denote by T_Δ . By Corollary 2.1(i), $F(T_2) = 8n - 14$. Further, we distinguish between two case.

Case 1. $(n-2) \bmod 2 = 0$.

By Corollary 2.1(i), we have that $F(T_3) = 14n - 26$. Since $(n-2) \bmod 2 = 0$, it follows that $(n-2) \bmod 3 \neq 0$, and by Corollary 2.1(ii), $F(T_4) = 22(n-1) - 21x + x^3$, where $x = 2$ or $x = 3$. For $n \geq 7$, $F(T_4) > F(T_3) > F(T_2)$ is satisfied.

Case 2. $(n-2) \bmod 2 \neq 0$.

By Corollary 2.1(ii), $F(T_3) = 14(n-1) - 13x + x^3$, where $x = 2$ or $x = 3$.

Subcase 2.1. $(n-2) \bmod 3 = 0$.

By Corollary 2.1(i), $F(T_4) = 22n - 42$. For $n \geq 7$ and $x = 2, 3$, it holds that $F(T_4) > F(T_3) > F(T_2)$.

Subcase 2.2. $(n-2) \bmod 3 \neq 0$.

By Corollary 2.1(ii), $F(T_4) = 22(n-1) - 21x + x^3$. Again, a straightforward calculation yields that $F(T_4) > F(T_3) > F(T_2)$.

So, we have shown that for $n \geq 3, 4, 5$ the tree with maximal F -index has maximal degree $n - 1$, and for $n \geq 5$ it has maximal degree $\Delta = 4$. Setting $\Delta = 4$ in Theorem 2.1 and Corollary 2.1, we complete the proof. \square

We would like to note that the results of Theorem 2.2 coincide with the results of Theorem 2.2 in [17], pertaining to the zeroth-order general Randić index of a graph, when $\alpha = 3$ and $m = n - 1$.

In the sequel we present some computational results obtain by integer linear programming and by exhaustive computer search of trees with maximal F -index.

2.3 Computational results

Degree sequences of trees with bounded maximal degree and maximal $F(T)$ can be completely described by solving the integer linear programming problem in Lemma 2.1. We denote the number of vertices of tree T of degree i by n_i , $\forall i = 1, 2, \dots, \Delta$ and the number of edges, connecting a vertex of degree i with a vertex of degree j , by m_{ij} .

Lemma 2.1. *Let T be a tree with maximal F -index among all trees with n vertices and maximal degree Δ . Then, the trees with maximal F -index are completely described by solving the maximization problem*

$$\begin{aligned}
& \text{maximize } F = \sum_{i=1}^{\Delta} i^3 n_i \\
& \text{subject to } \sum_{i=1}^{\Delta} n_i = n, \\
& \sum_{i=1}^{\Delta} i n_i = 2(n - 1), \\
& \sum_{i=2}^{\Delta-1} n_i \leq 1, \\
& \sum_{j=1, j \neq i}^{\Delta} m_{ij} + 2m_{ii} = i n_i \quad 1 \leq i \leq \Delta, \\
& 0 \leq n_i \leq n - 1, \quad 1 \leq i \leq \Delta, \\
& 0 \leq m_{ij} \leq n - 2, \quad 1 \leq i, j \leq \Delta.
\end{aligned}$$

For experimental proposes we first consider the molecular trees of orders $n = 4, \dots, 20$. In this case, the previous integer linear programming model can be represented as follows.

$$\left. \begin{array}{ll}
 \text{maximize} & F = n_1 + 8n_2 + 27n_3 + 64n_4 \\
 \text{s. t.} & \begin{array}{l}
 n_1 + n_2 + n_3 + n_4 = n, \\
 n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n-1), \\
 n_2 + n_3 \leq 1, \\
 -n_1 + m_{12} + m_{13} + m_{14} = 0, \\
 -2n_2 + m_{12} + 2m_{22} + m_{23} + m_{24} = 0, \\
 -3n_3 + m_{13} + m_{23} + 2m_{33} + m_{34} = 0, \\
 -4n_4 + m_{14} + m_{24} + m_{34} + 2m_{44} = 0, \\
 0 \leq n_i \leq n-1, \quad 0 \leq m_{ij} \leq n-2, \quad 1 \leq i \leq 4, \quad 1 \leq j \leq 4.
 \end{array}
 \end{array} \right\} \quad (1)$$

The above integer linear program was implemented in Matlab [23], and run on 2.3 GHz Intel Core i5 processor with 4GB 1333 MHz DDR3 RAM. Beside the degree sequence that maximize the F -index, it gives only one corresponding tree. However, for a given degree sequence there usually exist several non-isomorphic trees with the same degree sequence. In view of this, the degree sequence as well as all corresponding trees were obtained by exhaustive computer search using the mathematical software Sage [26]. In the contrast to the integer linear program that gives a solution for n of order 1000000 and $\Delta \leq 400$ in less than a minute, the exhaustive computer search with Sage for $n = 20$ took several hours. On the other hand, due to the closed-form solutions in Theorem 2.1, we obtain the degree sequence that maximizes the F -index for arbitrary n and arbitrary Δ in few milliseconds.

The experimental results for $\Delta = 4$ and $\Delta = 5$ are given in Tables 1 and 2, respectively, while their corresponding trees are given in Figures 1 and 2.

n	Sage		LP solution - Matlab							F
	$D(T)$	$\#T$	Non-zero variables							
4	$[3^1, 1^3]$	1	n_1 3	n_3 1		$m_{1,3}$ 3				30
5	$[4^1, 1^4]$	1	n_1 4	n_4 1		$m_{1,4}$ 4				68
6	$[4^1, 2^1, 1^4]$	1	n_1 4	n_2 1	n_4 1	$m_{1,2}$ 1	$m_{1,4}$ 3	$m_{2,4}$ 1		76
7	$[4^1, 3^1, 1^5]$	1	n_1 5	n_3 1	n_4 1	$m_{1,3}$ 2	$m_{1,4}$ 3	$m_{3,4}$ 1		96
8	$[4^2, 1^6]$	1	n_1 6	n_4 2		$m_{1,4}$ 6	$m_{4,4}$ 1			134
9	$[4^2, 2^1, 1^6]$	2	n_1 6	n_2 1	n_4 2	$m_{1,4}$ 6	$m_{2,4}$ 2			142
10	$[4^2, 3^1, 1^7]$	2	n_1 7	n_3 1	n_4 2	$m_{1,3}$ 1	$m_{1,4}$ 6	$m_{3,4}$ 2		162
11	$[4^3, 1^8]$	1	n_1 8	n_4 3		$m_{1,4}$ 8	$m_{4,4}$ 2			200
12	$[4^3, 2^1, 1^8]$	3	n_1 8	n_2 1	n_4 3	$m_{1,4}$ 8	$m_{2,4}$ 2	$m_{4,4}$ 1		208
13	$[4^3, 3^1, 1^9]$	4	n_1 9	n_3 1	n_4 3	$m_{1,4}$ 9	$m_{3,4}$ 3			228
14	$[4^4, 1^{10}]$	2	n_1 10	n_4 4		$m_{1,4}$ 10	$m_{4,4}$ 3			266
15	$[4^4, 2^1, 1^{10}]$	6	n_1 10	n_2 1	n_4 4	$m_{1,4}$ 10	$m_{2,4}$ 2	$m_{4,4}$ 2		274
16	$[4^4, 3^1, 1^{11}]$	8	n_1 11	n_3 1	n_4 4	$m_{1,4}$ 11	$m_{3,4}$ 3	$m_{4,4}$ 1		294
17	$[4^5, 1^{12}]$	3	n_1 12	n_4 5		$m_{1,4}$ 12	$m_{4,4}$ 4			332
18	$[4^5, 2^1, 1^{12}]$	14	n_1 12	n_2 1	n_4 5	$m_{1,4}$ 12	$m_{2,4}$ 2	$m_{4,4}$ 3		340
19	$[4^5, 3^1, 1^{13}]$	17	n_1 13	n_3 1	n_4 5	$m_{1,4}$ 13	$m_{3,4}$ 3	$m_{4,4}$ 2		360
20	$[4^6, 1^{14}]$	5	n_1 14	n_4 6		$m_{1,4}$ 14	$m_{4,4}$ 5			398

Table 1: Extremal molecular trees of order up to 20. First column: the order of a tree. Second column: the degree sequences that maximize the F -index and the number of corresponding trees, obtained by Sage. Third column: solutions of an integer linear programming problem with one realization of each degree sequence, obtained by Matlab. Fourt column: the value of the F -index.

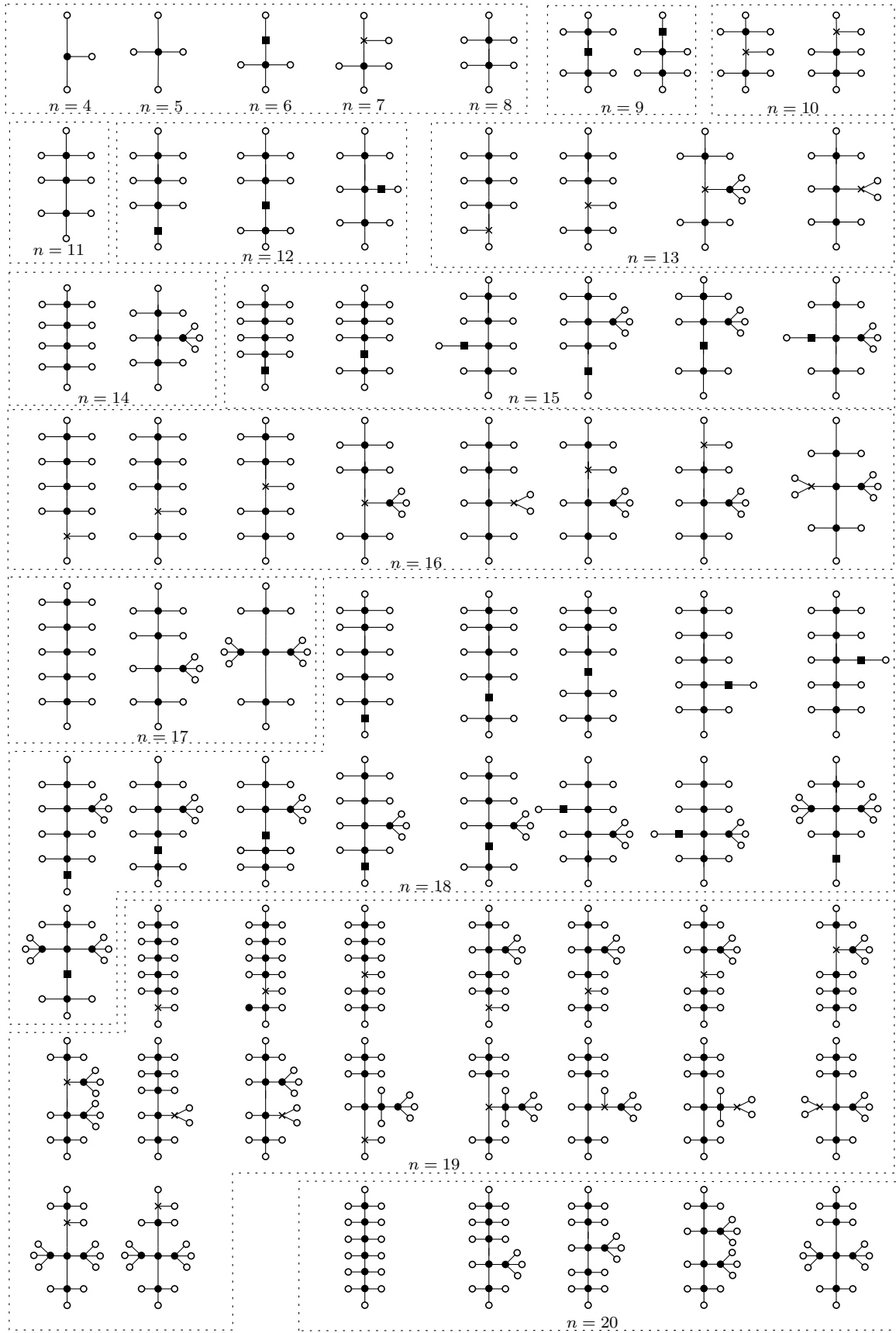


Figure 1: Extremal molecular trees of order $n = 4, \dots, 20$ with respect to the F -index.

n	Sage		LP solution - Matlab							F
	$D(T)$	$\#T$	Non-zero variables							
4	$[3^1, 1^3]$	1	n_1 3	n_3 1		$m_{1,3}$ 3				30
5	$[4^1, 1^4]$	1	n_1 4	n_4 1		$m_{1,4}$ 4				68
6	$[5^1, 1^5]$	1	n_1 5	n_5 1		$m_{1,5}$ 5				130
7	$[5^1, 2^1, 1^5]$	1	n_1 5	n_2 1	n_5 1	$m_{1,2}$ 1	$m_{1,5}$ 4	$m_{2,5}$ 1		138
8	$[5^1, 3^1, 1^6]$	1	n_1 6	n_3 1	n_5 1	$m_{1,3}$ 2	$m_{1,5}$ 4	$m_{3,5}$ 1		158
9	$[5^1, 4^1, 1^7]$	1	n_1 7	n_4 1	n_5 1	$m_{1,4}$ 3	$m_{1,5}$ 4	$m_{4,5}$ 1		196
10	$[5^2, 1^8]$	1	n_1 8	n_5 2		$m_{1,5}$ 8	$m_{5,5}$ 1			258
11	$[5^2, 2^1, 1^8]$	1	n_1 8	n_2 1	n_5 2	$m_{1,5}$ 8	$m_{2,5}$ 2			266
12	$[5^2, 3^1, 1^9]$	2	n_1 9	n_3 1	n_5 2	$m_{1,3}$ 2	$m_{1,5}$ 7	$m_{3,5}$ 1	$m_{5,5}$ 1	286
13	$[5^2, 4^1, 1^{10}]$	2	n_1 10	n_4 1	n_5 2	$m_{1,4}$ 2	$m_{1,5}$ 8	$m_{4,5}$ 2		324
14	$[5^3, 1^{11}]$	1	n_1 11	n_5 3		$m_{1,5}$ 11	$m_{5,5}$ 2			326
15	$[5^3, 2^1, 1^{11}]$	3	n_1 11	n_2 1	n_5 3	$m_{1,5}$ 11	$m_{2,5}$ 2	$m_{5,5}$ 1		394
16	$[5^3, 3^1, 1^{12}]$	4	n_1 12	n_3 1	n_5 3	$m_{1,3}$ 2	$m_{1,5}$ 10	$m_{3,5}$ 1	$m_{5,5}$ 2	414
17	$[5^3, 4^1, 1^{13}]$	4	n_1 13	n_4 1	n_5 3	$m_{1,4}$ 1	$m_{1,5}$ 12	$m_{4,5}$ 3		452
18	$[5^4, 1^{14}]$	2	n_1 14	n_5 4		$m_{1,5}$ 14	$m_{5,5}$ 3			514
19	$[5^4, 2^1, 1^{14}]$	7	n_1 14	n_2 1	n_5 4	$m_{1,2}$ 1	$m_{1,5}$ 13	$m_{2,5}$ 1	$m_{5,5}$ 3	522
20	$[5^4, 3^1, 1^{15}]$	8	n_1 15	n_3 1	n_5 4	$m_{1,3}$ 2	$m_{1,5}$ 13	$m_{3,5}$ 1	$m_{5,5}$ 3	542

Table 2: Extremal trees of order up to 20 and maximal degree $\Delta = 5$. First column: the order of a tree. Second column: the degree sequences that maximize the F -index and the number of corresponding trees, obtained by Sage. Third column: solutions of an integer linear programming problem with one realization of each degree sequence, obtained by Matlab. Fourt column: the value of the F -index.

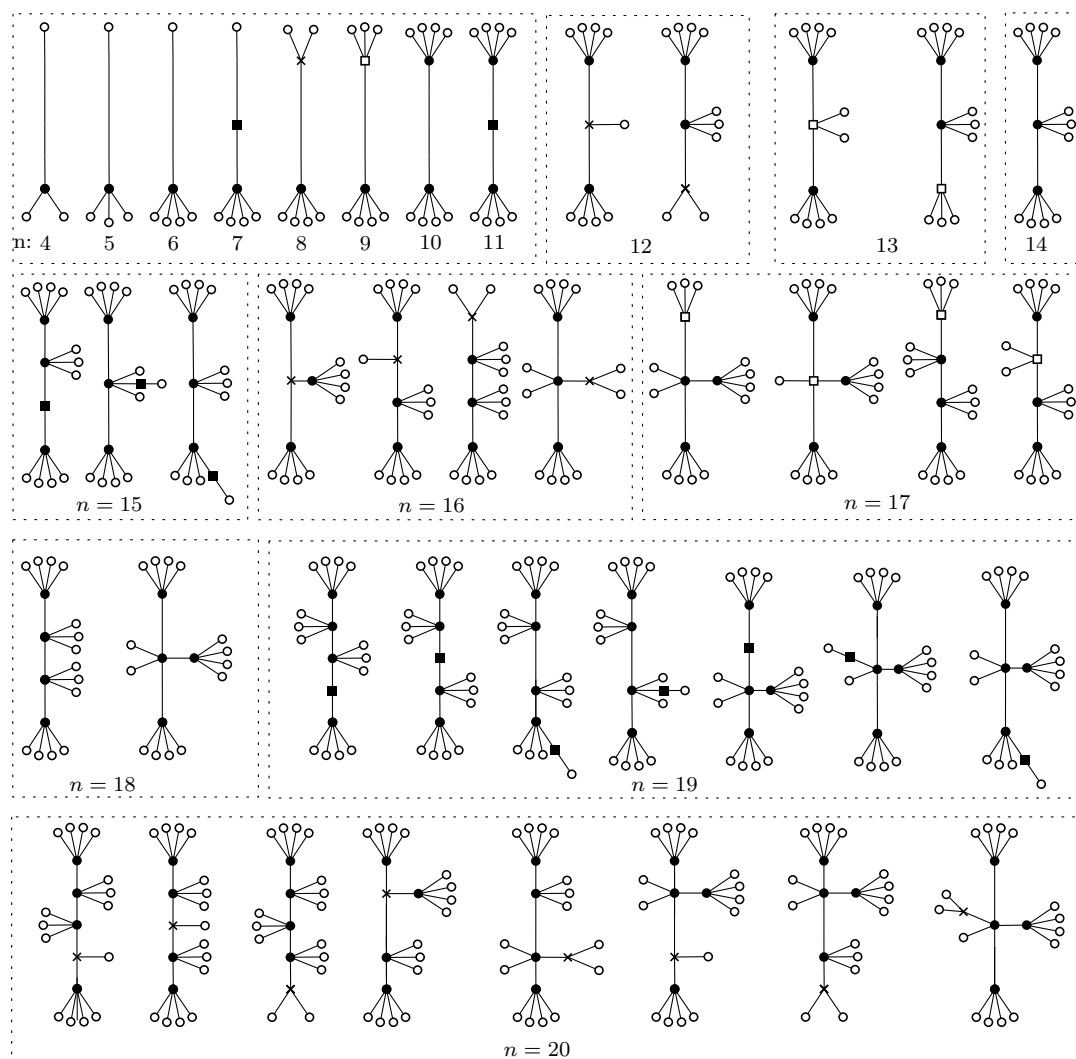


Figure 2: Extremal trees of order $n = 4, 5, \dots, 20$ and $\Delta = 5$ with respect to the F -index.

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